



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 05:56 PM JST

PDB ID : 7WTI
EMDB ID : EMD-32787
Title : SARS-CoV-2 Omicron variant spike in complex with Fab XGv264
Authors : Wang, X.; Fu, W.
Deposited on : 2022-02-04
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

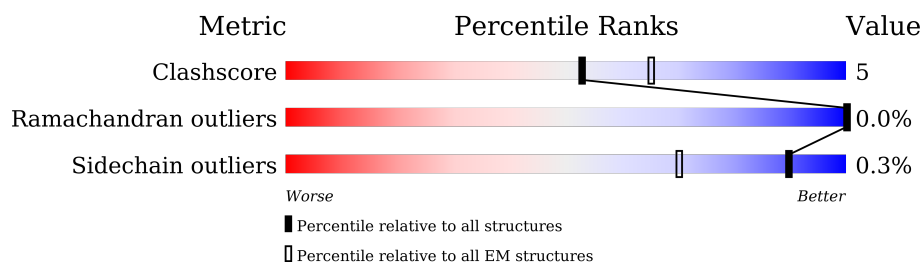
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



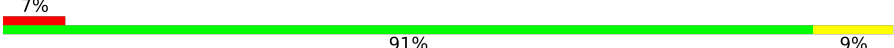
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1270	
1	B	1270	
1	C	1270	
2	G	118	
2	H	118	
2	I	118	
3	J	111	
3	K	111	

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Mol	Chain	Length	Quality of chain
3	L	111	 A horizontal bar chart showing the quality of chain L. The bar is divided into three segments: a red segment at the beginning labeled '7%', a green segment in the middle labeled '91%', and a yellow segment at the end labeled '9%'.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31536 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1098	Total	C	N	O	S	0	0
			8623	5520	1435	1629	39		
1	B	1098	Total	C	N	O	S	0	0
			8623	5520	1435	1629	39		
1	C	1098	Total	C	N	O	S	0	0
			8623	5520	1435	1629	39		

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	208	ILE	LEU	variant	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	212	PRO	-	insertion	UNP P0DTC2
A	213	GLU	-	insertion	UNP P0DTC2
A	341	ASP	GLY	variant	UNP P0DTC2
A	373	LEU	SER	variant	UNP P0DTC2
A	375	PRO	SER	variant	UNP P0DTC2
A	377	PHE	SER	variant	UNP P0DTC2
A	419	ASN	LYS	variant	UNP P0DTC2
A	442	LYS	ASN	variant	UNP P0DTC2
A	448	SER	GLY	variant	UNP P0DTC2
A	479	ASN	SER	variant	UNP P0DTC2
A	480	LYS	THR	variant	UNP P0DTC2
A	486	ALA	GLU	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	SER	GLY	variant	UNP P0DTC2
A	500	ARG	GLN	variant	UNP P0DTC2
A	503	TYR	ASN	variant	UNP P0DTC2
A	507	HIS	TYR	variant	UNP P0DTC2
A	549	LYS	THR	variant	UNP P0DTC2
A	616	GLY	ASP	variant	UNP P0DTC2
A	657	TYR	HIS	variant	UNP P0DTC2
A	681	LYS	ASN	variant	UNP P0DTC2
A	683	HIS	PRO	variant	UNP P0DTC2
A	685	ALA	ARG	engineered mutation	UNP P0DTC2
A	687	ALA	ARG	engineered mutation	UNP P0DTC2
A	766	LYS	ASN	variant	UNP P0DTC2
A	798	TYR	ASP	variant	UNP P0DTC2
A	819	PRO	PHE	engineered mutation	UNP P0DTC2
A	858	LYS	ASN	variant	UNP P0DTC2
A	894	PRO	ALA	engineered mutation	UNP P0DTC2
A	901	PRO	ALA	engineered mutation	UNP P0DTC2
A	944	PRO	ALA	engineered mutation	UNP P0DTC2
A	956	HIS	GLN	variant	UNP P0DTC2
A	971	LYS	ASN	variant	UNP P0DTC2
A	983	PHE	LEU	variant	UNP P0DTC2
A	988	PRO	LYS	engineered mutation	UNP P0DTC2
A	989	PRO	VAL	engineered mutation	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	208	ILE	LEU	variant	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	212	PRO	-	insertion	UNP P0DTC2
B	213	GLU	-	insertion	UNP P0DTC2
B	341	ASP	GLY	variant	UNP P0DTC2
B	373	LEU	SER	variant	UNP P0DTC2
B	375	PRO	SER	variant	UNP P0DTC2
B	377	PHE	SER	variant	UNP P0DTC2
B	419	ASN	LYS	variant	UNP P0DTC2
B	442	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	448	SER	GLY	variant	UNP P0DTC2
B	479	ASN	SER	variant	UNP P0DTC2
B	480	LYS	THR	variant	UNP P0DTC2
B	486	ALA	GLU	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	SER	GLY	variant	UNP P0DTC2
B	500	ARG	GLN	variant	UNP P0DTC2
B	503	TYR	ASN	variant	UNP P0DTC2
B	507	HIS	TYR	variant	UNP P0DTC2
B	549	LYS	THR	variant	UNP P0DTC2
B	616	GLY	ASP	variant	UNP P0DTC2
B	657	TYR	HIS	variant	UNP P0DTC2
B	681	LYS	ASN	variant	UNP P0DTC2
B	683	HIS	PRO	variant	UNP P0DTC2
B	685	ALA	ARG	engineered mutation	UNP P0DTC2
B	687	ALA	ARG	engineered mutation	UNP P0DTC2
B	766	LYS	ASN	variant	UNP P0DTC2
B	798	TYR	ASP	variant	UNP P0DTC2
B	819	PRO	PHE	engineered mutation	UNP P0DTC2
B	858	LYS	ASN	variant	UNP P0DTC2
B	894	PRO	ALA	engineered mutation	UNP P0DTC2
B	901	PRO	ALA	engineered mutation	UNP P0DTC2
B	944	PRO	ALA	engineered mutation	UNP P0DTC2
B	956	HIS	GLN	variant	UNP P0DTC2
B	971	LYS	ASN	variant	UNP P0DTC2
B	983	PHE	LEU	variant	UNP P0DTC2
B	988	PRO	LYS	engineered mutation	UNP P0DTC2
B	989	PRO	VAL	engineered mutation	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	208	ILE	LEU	variant	UNP P0DTC2
C	211	GLU	-	insertion	UNP P0DTC2
C	212	PRO	-	insertion	UNP P0DTC2
C	213	GLU	-	insertion	UNP P0DTC2
C	341	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	LEU	SER	variant	UNP P0DTC2
C	375	PRO	SER	variant	UNP P0DTC2
C	377	PHE	SER	variant	UNP P0DTC2
C	419	ASN	LYS	variant	UNP P0DTC2
C	442	LYS	ASN	variant	UNP P0DTC2
C	448	SER	GLY	variant	UNP P0DTC2
C	479	ASN	SER	variant	UNP P0DTC2
C	480	LYS	THR	variant	UNP P0DTC2
C	486	ALA	GLU	variant	UNP P0DTC2
C	495	ARG	GLN	variant	UNP P0DTC2
C	498	SER	GLY	variant	UNP P0DTC2
C	500	ARG	GLN	variant	UNP P0DTC2
C	503	TYR	ASN	variant	UNP P0DTC2
C	507	HIS	TYR	variant	UNP P0DTC2
C	549	LYS	THR	variant	UNP P0DTC2
C	616	GLY	ASP	variant	UNP P0DTC2
C	657	TYR	HIS	variant	UNP P0DTC2
C	681	LYS	ASN	variant	UNP P0DTC2
C	683	HIS	PRO	variant	UNP P0DTC2
C	685	ALA	ARG	engineered mutation	UNP P0DTC2
C	687	ALA	ARG	engineered mutation	UNP P0DTC2
C	766	LYS	ASN	variant	UNP P0DTC2
C	798	TYR	ASP	variant	UNP P0DTC2
C	819	PRO	PHE	engineered mutation	UNP P0DTC2
C	858	LYS	ASN	variant	UNP P0DTC2
C	894	PRO	ALA	engineered mutation	UNP P0DTC2
C	901	PRO	ALA	engineered mutation	UNP P0DTC2
C	944	PRO	ALA	engineered mutation	UNP P0DTC2
C	956	HIS	GLN	variant	UNP P0DTC2
C	971	LYS	ASN	variant	UNP P0DTC2
C	983	PHE	LEU	variant	UNP P0DTC2
C	988	PRO	LYS	engineered mutation	UNP P0DTC2
C	989	PRO	VAL	engineered mutation	UNP P0DTC2

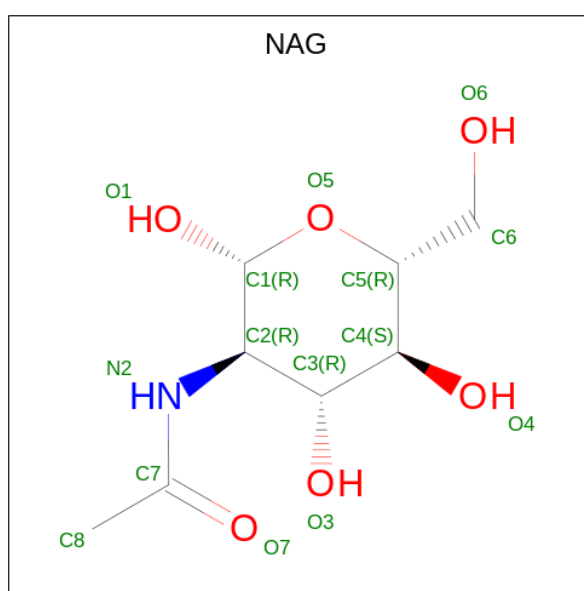
- Molecule 2 is a protein called Heavy chain of XGv264.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	118	Total	C	N	O	S	0	0
			912	589	149	169	5		
2	I	118	Total	C	N	O	S	0	0
			912	589	149	169	5		
2	G	118	Total	C	N	O	S	0	0
			912	589	149	169	5		

- Molecule 3 is a protein called Light chain of XGv264.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	111	Total	C	N	O	S	0	0
			809	504	135	167	3		
3	L	111	Total	C	N	O	S	0	0
			809	504	135	167	3		
3	J	111	Total	C	N	O	S	0	0
			809	504	135	167	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

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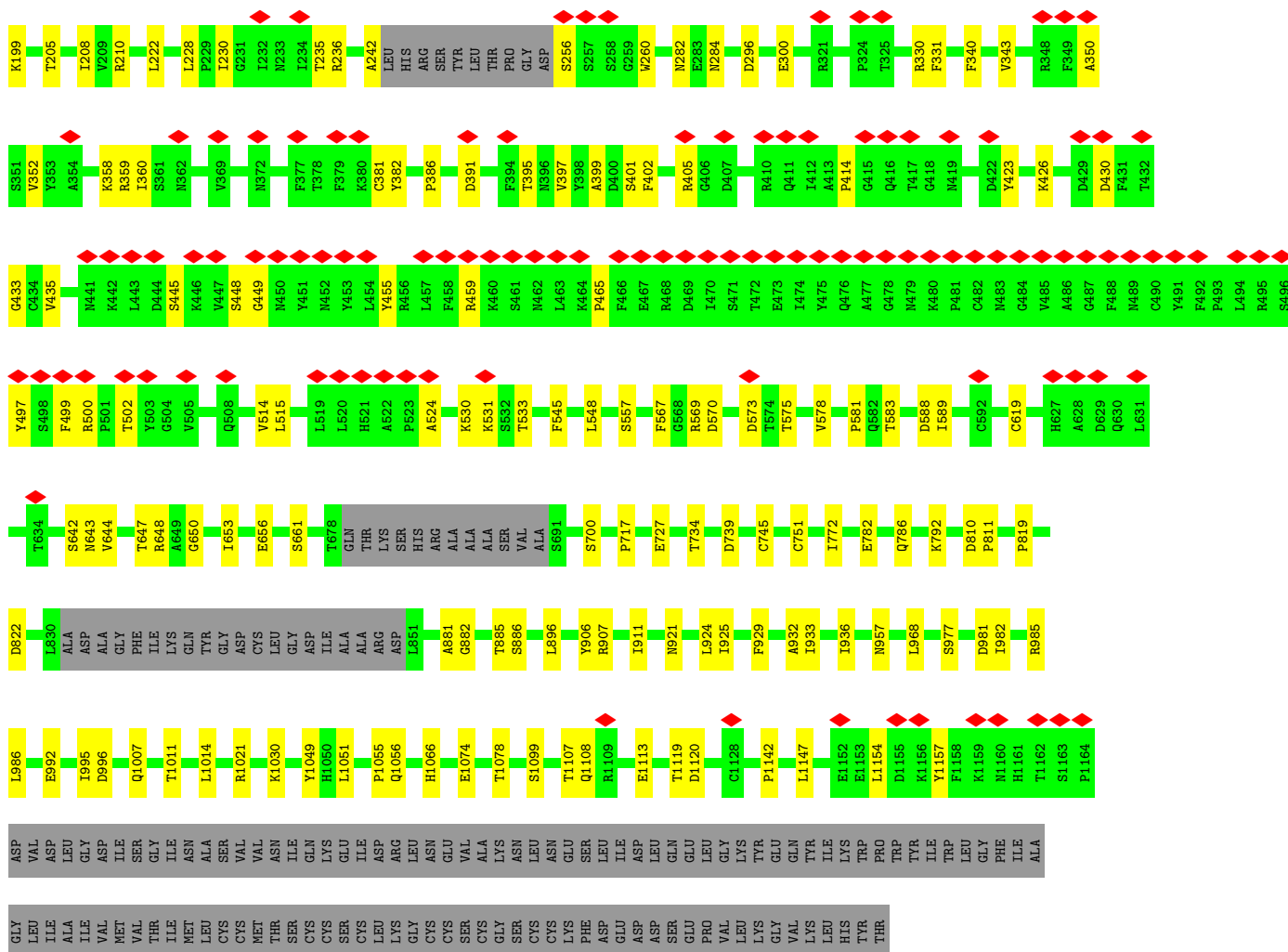
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

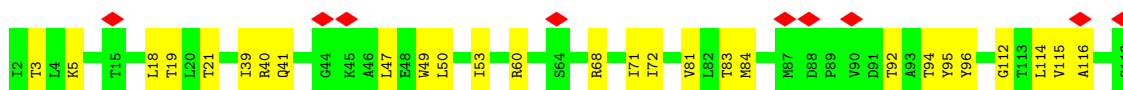
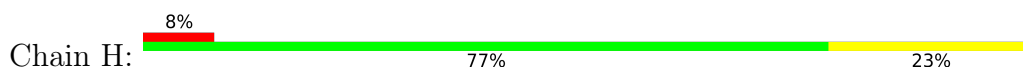
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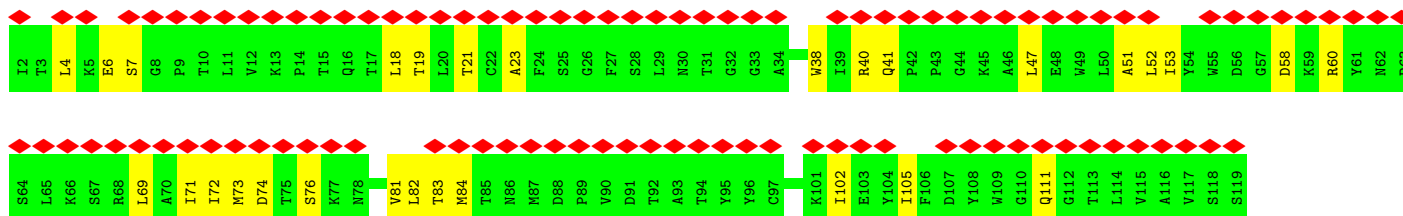
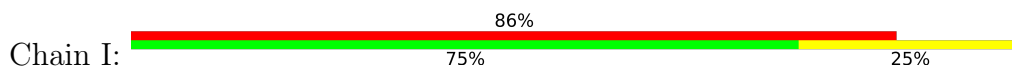
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	



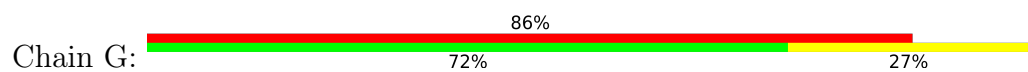
• Molecule 2: Heavy chain of XGv264



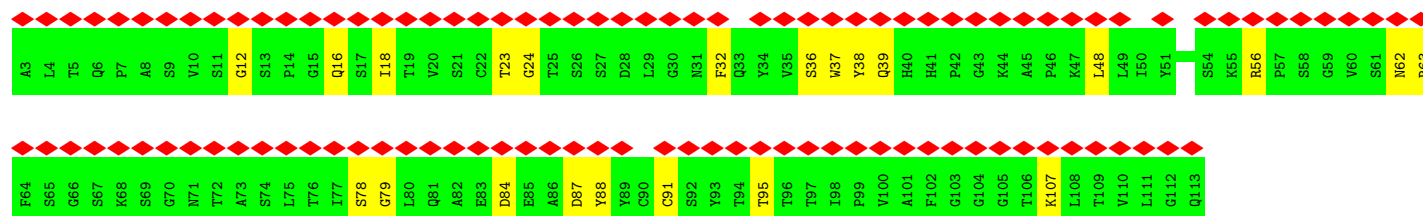
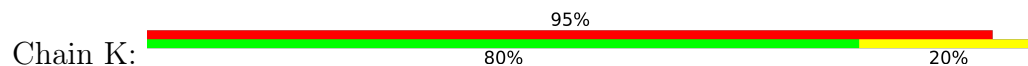
• Molecule 2: Heavy chain of XGv264



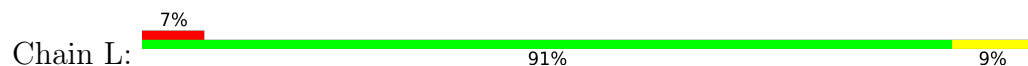
• Molecule 2: Heavy chain of XGv264



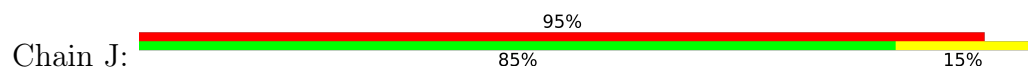
• Molecule 3: Light chain of XGv264



• Molecule 3: Light chain of XGv264



• Molecule 3: Light chain of XGv264



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	494849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	2.976	Depositor
Minimum map value	-1.561	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/8832	0.56	0/12021
1	B	0.28	0/8832	0.58	1/12021 (0.0%)
1	C	0.28	0/8832	0.59	4/12021 (0.0%)
2	G	0.28	0/936	0.67	1/1277 (0.1%)
2	H	0.28	0/936	0.66	0/1277
2	I	0.29	0/936	0.69	2/1277 (0.2%)
3	J	0.26	0/827	0.58	0/1127
3	K	0.28	0/827	0.67	0/1127
3	L	0.26	0/827	0.60	0/1127
All	All	0.28	0/31785	0.59	8/43275 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
2	I	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	996	ASP	CB-CG-OD1	8.33	125.80	118.30
1	C	173	LEU	CA-CB-CG	6.12	129.37	115.30
1	C	1147	LEU	CA-CB-CG	5.66	128.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	87	MET	C-N-CA	5.55	135.57	121.70
1	B	333	ASN	CB-CA-C	-5.52	99.36	110.40
2	I	73	MET	CA-CB-CG	5.14	122.03	113.30
1	C	996	ASP	CB-CG-OD2	-5.08	113.72	118.30
2	I	52	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	619	CYS	Peptide
1	B	446	LYS	Peptide
1	C	619	CYS	Peptide
2	I	40	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8623	0	8430	75	0
1	B	8623	0	8430	81	0
1	C	8623	0	8430	99	0
2	G	912	0	901	20	0
2	H	912	0	901	15	0
2	I	912	0	901	17	0
3	J	809	0	773	9	0
3	K	809	0	773	14	0
3	L	809	0	773	6	0
4	A	168	0	156	1	0
4	B	168	0	156	0	0
4	C	168	0	156	0	0
All	All	31536	0	30780	320	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:GLY:HA2	1:B:191:PHE:O	1.63	0.98
1:A:96:GLU:O	1:A:185:ASN:HB2	1.78	0.80
1:B:67:VAL:O	1:B:265:ALA:HB3	1.85	0.77
2:I:4:LEU:HA	2:I:23:ALA:O	1.86	0.74
2:I:18:LEU:O	2:I:83:THR:HA	1.96	0.66
1:C:449:GLY:HA2	1:C:499:PHE:H	1.63	0.64
1:C:126:VAL:HG23	1:C:171:PRO:HA	1.81	0.63
1:B:139:PRO:HG2	1:B:156:VAL:HG13	1.81	0.63
1:C:118:LEU:O	1:C:128:ILE:HA	1.99	0.62
1:C:143:HIS:HB3	1:C:260:TRP:HB2	1.82	0.61
1:B:130:VAL:HB	1:B:165:PHE:HB3	1.82	0.61
1:A:110:LEU:HD12	1:A:236:ARG:HH12	1.65	0.61
1:B:136:CYS:HB2	1:B:139:PRO:HG3	1.83	0.60
3:K:37:TRP:HE1	3:K:88:TYR:HB3	1.67	0.59
1:C:358:LYS:HB3	1:C:399:ALA:HB3	1.84	0.59
3:K:38:TYR:HB2	3:K:48:LEU:HG	1.84	0.59
3:J:37:TRP:HB2	3:J:50:ILE:HB	1.83	0.59
2:G:53:ILE:HD11	2:G:71:ILE:HG13	1.85	0.58
2:H:18:LEU:HD11	2:H:115:VAL:HG21	1.84	0.58
1:C:235:THR:HG23	1:C:236:ARG:HG3	1.86	0.58
1:C:782:GLU:O	1:C:786:GLN:NE2	2.37	0.58
1:B:583:THR:HB	1:B:585:GLU:OE1	2.04	0.57
1:C:644:VAL:HG12	1:C:653:ILE:HG22	1.86	0.57
1:B:353:TYR:HE1	1:B:456:ARG:HE	1.53	0.57
2:G:52:LEU:HD11	2:G:60:ARG:HD2	1.85	0.57
1:A:34:ARG:HD2	1:A:215:LEU:HD21	1.85	0.57
1:B:230:ILE:HG22	1:B:232:ILE:H	1.70	0.57
2:G:13:LYS:HB2	2:G:16:GLN:HB2	1.86	0.56
1:A:911:ILE:HD12	1:A:1049:TYR:HB3	1.87	0.56
2:G:72:ILE:HB	2:G:81:VAL:HB	1.87	0.56
1:A:128:ILE:HB	1:A:167:TYR:HB3	1.87	0.56
1:C:208:ILE:HD12	1:C:210:ARG:HH21	1.70	0.56
1:A:502:THR:HB	3:L:30:GLY:HA3	1.86	0.56
1:B:454:LEU:HB3	1:B:494:LEU:HD12	1.86	0.56
1:A:43:PHE:HB3	1:B:568:GLY:HA2	1.85	0.56
1:B:190:VAL:HB	1:B:201:TYR:HB2	1.88	0.56
1:C:24:LEU:HG	1:C:78:ARG:HH11	1.71	0.56
2:G:21:THR:HG22	2:G:81:VAL:HG22	1.88	0.55
1:C:545:PHE:HB2	1:C:548:LEU:HD12	1.88	0.55
1:B:66:HIS:O	1:B:78:ARG:NH1	2.38	0.55
1:B:600:ILE:HB	1:B:611:ALA:HB3	1.87	0.55
1:C:435:VAL:HG12	1:C:514:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ALA:O	1:A:636:ARG:NH2	2.35	0.55
1:A:782:GLU:OE2	1:A:1021:ARG:NH1	2.40	0.55
1:C:405:ARG:HH21	1:C:497:TYR:HA	1.72	0.55
2:H:53:ILE:HD11	2:H:71:ILE:HG13	1.89	0.55
1:A:1145:PRO:HA	1:A:1148:ASP:HB2	1.89	0.55
1:C:557:SER:HB3	1:C:588:ASP:HB2	1.89	0.54
1:B:31:SER:O	1:B:59:PHE:HA	2.07	0.54
1:B:426:LYS:HE2	1:B:465:PRO:HG3	1.89	0.54
1:B:456:ARG:HD3	1:B:459:ARG:HG3	1.90	0.54
1:C:1108:GLN:NE2	1:C:1113:GLU:OE1	2.41	0.54
1:B:821:GLU:HA	1:B:824:LEU:HD12	1.88	0.54
2:I:51:ALA:HB2	2:I:69:LEU:HD21	1.90	0.54
1:B:536:VAL:HG11	1:B:539:LYS:HE2	1.90	0.54
1:B:635:TRP:HB2	1:B:638:TYR:HB2	1.89	0.54
3:K:39:GLN:HA	3:K:87:ASP:O	2.08	0.54
1:C:929:PHE:O	1:C:932:ALA:HB3	2.08	0.54
2:H:68:ARG:NH2	2:H:84:MET:SD	2.81	0.54
1:B:502:THR:HB	3:J:30:GLY:HA3	1.90	0.53
1:C:152:SER:OG	1:C:153:GLU:OE1	2.25	0.53
2:I:58:ASP:OD2	2:I:60:ARG:NH1	2.41	0.53
1:B:1095:GLY:HA2	1:B:1109:ARG:HG3	1.90	0.53
1:C:186:LEU:HB2	1:C:205:THR:HB	1.90	0.53
1:A:987:ASP:HB2	1:A:989:PRO:HD2	1.90	0.53
1:B:67:VAL:HA	1:B:78:ARG:HD2	1.91	0.53
1:B:100:ILE:O	1:B:242:ALA:N	2.41	0.53
1:C:98:SER:HA	1:C:178:GLY:HA3	1.90	0.53
2:G:95:TYR:O	2:G:112:GLY:CA	2.57	0.53
1:C:734:THR:OG1	1:C:957:ASN:ND2	2.42	0.53
1:B:782:GLU:O	1:B:786:GLN:NE2	2.42	0.53
2:G:19:THR:HG22	2:G:83:THR:HG22	1.91	0.52
1:A:1019:GLU:OE1	1:C:1021:ARG:NH1	2.41	0.52
1:A:102:ARG:NH1	1:A:122:ASN:O	2.43	0.52
1:A:565:GLN:NE2	1:C:42:VAL:O	2.42	0.52
1:A:642:SER:OG	1:A:643:ASN:N	2.43	0.52
1:B:916:ASN:ND2	1:B:1113:GLU:OE2	2.42	0.52
1:C:907:ARG:NH1	1:C:1051:LEU:O	2.43	0.52
1:B:184:LYS:HE2	1:B:209:VAL:HG22	1.91	0.51
2:G:18:LEU:O	2:G:83:THR:HA	2.11	0.51
1:C:359:ARG:NH2	1:C:360:ILE:O	2.39	0.51
1:C:455:TYR:HB3	1:C:497:TYR:HE1	1.75	0.51
1:A:706:SER:HB3	1:C:792:LYS:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ILE:O	1:C:77:LYS:N	2.44	0.51
1:C:97:LYS:HB2	1:C:183:PHE:HA	1.93	0.51
1:C:445:SER:HB3	2:I:102:ILE:HD12	1.92	0.51
2:H:19:THR:HG22	2:H:83:THR:HG22	1.92	0.51
2:H:39:ILE:HG13	2:H:49:TRP:HA	1.91	0.51
1:B:336:ASN:O	1:B:363:CYS:HB2	2.11	0.51
1:B:441:ASN:O	1:B:445:SER:OG	2.27	0.51
1:B:1146:GLU:HB2	1:B:1150:PHE:HB2	1.92	0.51
1:B:754:LEU:O	1:B:757:GLN:NE2	2.45	0.50
1:C:350:ALA:HB3	1:C:401:SER:HB2	1.92	0.50
3:J:63:ARG:NH1	3:J:84:ASP:OD2	2.45	0.50
3:J:89:TYR:HD1	3:J:103:GLY:HA3	1.77	0.50
1:C:433:GLY:HA3	1:C:515:LEU:O	2.12	0.50
1:B:128:ILE:HD13	1:B:167:TYR:HD2	1.76	0.50
1:A:209:VAL:HG13	1:A:210:ARG:HE	1.75	0.50
1:B:456:ARG:NH1	1:B:458:PHE:O	2.45	0.50
3:K:56:ARG:HD3	3:K:62:ASN:HA	1.94	0.50
3:L:24:GLY:O	3:L:71:ASN:ND2	2.45	0.50
1:A:500:ARG:O	1:A:502:THR:N	2.42	0.50
1:C:647:THR:OG1	1:C:650:GLY:O	2.27	0.50
3:J:79:GLY:O	3:J:81:GLN:NE2	2.45	0.50
1:C:110:LEU:HA	1:C:135:PHE:HD2	1.77	0.49
2:G:87:MET:N	2:G:87:MET:SD	2.85	0.49
1:B:607:SER:OG	1:B:608:ASN:N	2.45	0.49
3:J:24:GLY:O	3:J:71:ASN:ND2	2.44	0.49
1:C:569:ARG:NH1	1:C:573:ASP:OD1	2.43	0.49
3:K:16:GLN:HG3	3:K:79:GLY:H	1.76	0.49
1:A:881:ALA:O	1:A:885:THR:OG1	2.31	0.49
1:B:77:LYS:N	1:B:260:TRP:O	2.45	0.49
1:C:330:ARG:HE	1:C:581:PRO:HD2	1.76	0.49
1:C:531:LYS:NZ	1:C:533:THR:OG1	2.44	0.48
1:A:329:VAL:HG12	1:A:544:ASN:HB3	1.94	0.48
1:B:341:ASP:OD1	1:B:341:ASP:N	2.46	0.48
1:B:459:ARG:NH1	1:B:461:SER:O	2.45	0.48
1:A:1108:GLN:NE2	1:A:1113:GLU:OE1	2.45	0.48
1:C:567:PHE:HA	1:C:578:VAL:HG12	1.94	0.48
1:C:1055:PRO:O	1:C:1056:GLN:NE2	2.43	0.48
3:L:41:HIS:HB2	3:L:44:LYS:HB2	1.95	0.48
1:A:444:ASP:OD2	1:A:511:ARG:NE	2.42	0.48
1:C:109:THR:HG23	1:C:111:ASP:H	1.78	0.48
2:I:41:GLN:HA	2:I:47:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:ASP:OD1	1:C:430:ASP:N	2.45	0.48
2:H:40:ARG:HD3	2:H:50:LEU:HD11	1.94	0.48
1:C:37:TYR:HB3	1:C:222:LEU:HB2	1.96	0.48
2:I:72:ILE:HB	2:I:81:VAL:HB	1.96	0.48
2:H:41:GLN:HB3	2:H:47:LEU:HD13	1.96	0.48
2:G:40:ARG:HE	2:G:50:LEU:HD11	1.79	0.48
1:C:228:LEU:HG	1:C:230:ILE:HG12	1.95	0.47
2:I:19:THR:HG22	2:I:83:THR:HG22	1.96	0.47
3:K:84:ASP:OD1	3:K:84:ASP:N	2.48	0.47
1:B:213:GLU:O	1:B:268:TYR:OH	2.31	0.47
2:G:4:LEU:HA	2:G:23:ALA:O	2.14	0.47
1:A:963:THR:O	1:A:967:GLN:NE2	2.47	0.47
1:C:382:TYR:HD2	1:C:414:PRO:HD2	1.78	0.47
1:A:987:ASP:OD1	1:A:987:ASP:N	2.47	0.47
1:B:282:ASN:OD1	1:B:286:THR:N	2.46	0.47
1:B:131:CYS:SG	1:B:132:GLU:N	2.87	0.47
1:B:658:VAL:HG23	1:B:697:TYR:HB3	1.97	0.47
1:C:982:ILE:HA	1:C:985:ARG:HG2	1.96	0.47
2:G:39:ILE:HG13	2:G:49:TRP:HA	1.95	0.47
1:A:992:GLU:HA	1:A:995:ILE:HG12	1.96	0.47
1:A:1159:LYS:O	1:A:1163:SER:OG	2.31	0.47
1:B:105:ILE:HB	1:B:238:GLN:HB2	1.96	0.47
1:B:140:PHE:CD1	1:B:143:HIS:HE1	2.33	0.47
2:H:72:ILE:HB	2:H:81:VAL:HB	1.95	0.47
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.97	0.47
1:C:992:GLU:HA	1:C:995:ILE:HG22	1.97	0.47
3:L:32:PHE:HZ	3:L:73:ALA:HB2	1.80	0.47
1:B:1021:ARG:NH1	1:B:1025:ASN:OD1	2.48	0.46
1:C:391:ASP:N	1:C:391:ASP:OD1	2.48	0.46
1:A:95:ILE:HG22	1:A:183:PHE:HB2	1.98	0.46
1:A:186:LEU:HB2	1:A:208:ILE:HD11	1.96	0.46
1:C:661:SER:HB2	1:C:700:SER:HB3	1.97	0.46
1:A:677:GLN:NE2	1:A:678:THR:O	2.48	0.46
1:B:642:SER:OG	1:B:643:ASN:N	2.49	0.46
1:A:101:ILE:HA	1:A:241:LEU:HA	1.97	0.46
1:A:503:TYR:HB3	1:A:507:HIS:HB2	1.97	0.46
1:C:739:ASP:OD1	1:C:739:ASP:N	2.46	0.46
1:A:34:ARG:NH1	1:A:188:GLU:OE2	2.47	0.46
1:A:1088:LYS:HA	1:A:1127:ASN:HA	1.98	0.46
1:C:717:PRO:HA	1:C:1074:GLU:HA	1.98	0.46
1:C:1120:ASP:OD1	1:C:1120:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:THR:HB	2:H:116:ALA:HA	1.96	0.46
1:A:1021:ARG:O	1:A:1025:ASN:ND2	2.48	0.46
1:C:282:ASN:HD21	1:C:284:ASN:HB2	1.81	0.46
2:I:6:GLU:O	2:I:111:GLN:NE2	2.49	0.46
1:B:813:LYS:HG3	1:B:815:SER:H	1.81	0.46
1:C:727:GLU:OE1	1:C:1066:HIS:NE2	2.46	0.46
1:B:366:ASP:OD1	1:B:366:ASP:N	2.47	0.45
1:B:396:ASN:C	1:B:396:ASN:HD22	2.18	0.45
1:C:381:CYS:H	1:C:386:PRO:HG3	1.80	0.45
1:B:296:ASP:N	1:B:296:ASP:OD1	2.48	0.45
1:C:502:THR:HA	3:K:32:PHE:HB2	1.96	0.45
1:A:14:GLN:HG3	1:A:153:GLU:HG3	1.99	0.45
1:A:668:ILE:HB	1:A:673:CYS:HA	1.99	0.45
1:C:578:VAL:HG22	1:C:589:ILE:HD11	1.97	0.45
1:C:1107:THR:OG1	1:C:1108:GLN:N	2.49	0.45
1:A:366:ASP:OD1	1:A:366:ASP:N	2.47	0.45
1:A:907:ARG:O	1:A:1038:GLN:NE2	2.50	0.45
1:C:330:ARG:HH22	1:C:583:THR:HG22	1.81	0.45
1:C:340:PHE:HA	1:C:343:VAL:HG22	1.98	0.45
1:C:642:SER:OG	1:C:656:GLU:OE2	2.35	0.45
1:B:422:ASP:OD1	1:B:422:ASP:N	2.47	0.45
1:B:911:ILE:HD12	1:B:1049:TYR:HB3	1.99	0.45
3:K:36:SER:OG	3:K:91:CYS:SG	2.74	0.45
1:C:426:LYS:HG2	1:C:465:PRO:HG3	1.97	0.45
2:H:21:THR:HG22	2:H:81:VAL:HG22	1.98	0.45
1:A:606:THR:HG22	1:A:607:SER:H	1.82	0.45
1:A:1039:SER:OG	1:A:1045:CYS:SG	2.70	0.45
1:B:21:ARG:HE	1:B:22:THR:H	1.65	0.45
1:C:330:ARG:HH21	1:C:581:PRO:HD2	1.81	0.45
1:B:441:ASN:HA	1:B:509:PRO:HG2	1.99	0.45
2:I:7:SER:OG	2:I:21:THR:OG1	2.34	0.45
1:C:772:ILE:HD11	1:C:1014:LEU:HD22	1.98	0.45
1:A:446:LYS:HD2	1:A:450:ASN:HA	1.98	0.44
1:C:448:SER:OG	2:I:60:ARG:NE	2.44	0.44
1:B:1045:CYS:O	1:B:1066:HIS:ND1	2.50	0.44
1:C:296:ASP:O	1:C:300:GLU:N	2.48	0.44
1:C:911:ILE:HD12	1:C:1049:TYR:HB3	1.98	0.44
2:G:41:GLN:HB2	2:G:47:LEU:HD13	1.98	0.44
1:A:330:ARG:NH1	1:A:582:GLN:OE1	2.49	0.44
1:C:882:GLY:O	1:C:886:SER:OG	2.30	0.44
2:I:38:TRP:CD2	2:I:82:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:MET:HG3	1:B:152:SER:H	1.82	0.44
1:B:592:CYS:HA	1:B:593:SER:HA	1.76	0.44
1:B:881:ALA:O	1:B:885:THR:OG1	2.36	0.44
1:A:450:ASN:HD21	1:A:453:TYR:HD2	1.66	0.44
1:C:548:LEU:HD22	1:C:575:THR:HG21	2.00	0.44
2:I:21:THR:HG22	2:I:81:VAL:HG22	1.99	0.44
3:K:23:THR:OG1	3:K:24:GLY:N	2.50	0.44
1:A:22:THR:HG21	1:A:78:ARG:HG3	2.00	0.44
1:A:338:CYS:HB3	1:A:363:CYS:HB3	1.81	0.44
1:B:914:THR:OG1	1:B:915:GLN:N	2.50	0.44
1:B:126:VAL:HB	1:B:169:SER:O	2.18	0.44
1:C:118:LEU:HB3	1:C:129:LYS:HB2	2.00	0.44
1:C:881:ALA:O	1:C:885:THR:OG1	2.26	0.44
1:A:610:VAL:O	1:A:638:TYR:OH	2.34	0.44
1:B:236:ARG:HD3	1:B:238:GLN:HE22	1.82	0.44
2:G:94:THR:HA	2:G:114:LEU:HA	1.99	0.44
1:A:282:ASN:HD21	1:A:284:ASN:HB2	1.83	0.44
3:K:12:GLY:HA3	3:K:18:ILE:HD13	2.00	0.44
1:A:22:THR:HB	1:A:24:LEU:HD23	2.00	0.43
1:B:93:ALA:HB1	1:B:186:LEU:HD11	2.00	0.43
1:C:968:LEU:O	1:C:977:SER:OG	2.31	0.43
1:A:570:ASP:OD1	1:A:570:ASP:N	2.50	0.43
1:C:933:ILE:HD12	1:C:936:ILE:HG13	2.00	0.43
1:B:353:TYR:HD1	1:B:456:ARG:HB2	1.83	0.43
1:B:411:GLN:HE22	1:B:420:ILE:H	1.67	0.43
1:A:326:GLU:HG3	1:A:541:VAL:HG23	2.00	0.43
1:B:982:ILE:HG23	1:B:986:LEU:HD12	2.00	0.43
3:L:56:ARG:NH1	3:L:61:SER:O	2.42	0.43
2:G:95:TYR:O	2:G:112:GLY:HA3	2.18	0.43
1:A:97:LYS:HB2	1:A:183:PHE:HA	2.01	0.43
1:C:352:VAL:HA	1:C:402:PHE:HD1	1.83	0.43
1:A:130:VAL:HG21	1:A:230:ILE:HG12	2.00	0.43
1:A:717:PRO:HA	1:A:1074:GLU:HA	2.00	0.43
1:B:44:ARG:HG3	1:C:569:ARG:HB2	2.00	0.43
2:G:95:TYR:O	2:G:112:GLY:HA2	2.19	0.43
1:C:727:GLU:OE2	1:C:1030:LYS:NZ	2.43	0.43
1:A:43:PHE:N	1:B:567:PHE:O	2.48	0.43
2:I:53:ILE:HG12	2:I:71:ILE:HG21	2.00	0.43
2:I:105:ILE:HD13	3:K:36:SER:HB3	2.00	0.43
1:A:715:ALA:HB3	1:C:896:LEU:HB3	2.01	0.42
1:A:1095:GLY:O	1:C:906:TYR:OH	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:ASP:O	1:B:991:ALA:N	2.47	0.42
1:C:68:ILE:N	1:C:78:ARG:O	2.51	0.42
1:C:1007:GLN:O	1:C:1011:THR:OG1	2.29	0.42
1:A:1118:THR:HB	1:A:1142:PRO:HD3	2.01	0.42
1:B:297:PRO:HG2	1:B:610:VAL:HG21	2.01	0.42
1:B:360:ILE:HB	1:B:397:VAL:HG23	2.01	0.42
1:C:35:GLY:HA3	1:C:56:LEU:HB3	2.02	0.42
1:A:1141:ASP:HB3	1:A:1144:GLN:HB2	2.01	0.42
2:H:96:TYR:HD1	2:H:112:GLY:HA3	1.85	0.42
1:C:981:ASP:OD1	1:C:981:ASP:N	2.50	0.42
1:A:765:LEU:HD12	1:A:1010:VAL:HG21	2.00	0.42
1:C:192:LYS:HE2	1:C:199:LYS:HD2	2.01	0.42
1:C:423:TYR:HB3	1:C:459:ARG:HG2	2.01	0.42
1:C:745:CYS:HB3	1:C:751:CYS:HB3	1.52	0.42
1:B:576:ASP:OD1	1:B:576:ASP:N	2.52	0.42
1:B:1084:CYS:SG	1:B:1088:LYS:N	2.93	0.42
1:C:1078:THR:O	1:C:1099:SER:OG	2.32	0.42
1:A:40:ASP:OD1	1:A:40:ASP:N	2.51	0.42
1:A:184:LYS:HA	1:A:208:ILE:HB	2.01	0.42
1:A:460:LYS:HD2	1:A:460:LYS:HA	1.90	0.42
1:A:973:GLY:O	1:A:997:ARG:NH1	2.53	0.42
1:C:500:ARG:NH2	3:K:95:THR:OG1	2.51	0.42
1:C:810:ASP:HA	1:C:811:PRO:HD3	1.89	0.42
2:G:99:HIS:HB3	2:G:107:ASP:HB3	2.01	0.42
1:B:554:LEU:HD12	1:B:587:LEU:HD13	2.00	0.42
1:C:570:ASP:OD1	1:C:570:ASP:N	2.51	0.42
3:L:50:ILE:HD13	3:L:50:ILE:HA	1.96	0.42
1:B:1119:THR:OG1	1:B:1140:TYR:O	2.34	0.42
1:B:116:SER:HB2	1:B:133:PHE:HD2	1.85	0.41
1:B:1160:ASN:OD1	1:B:1160:ASN:N	2.51	0.41
1:C:359:ARG:HH22	1:C:397:VAL:H	1.66	0.41
1:A:963:THR:HA	1:A:966:LYS:HE2	2.02	0.41
2:G:65:LEU:HD12	2:G:68:ARG:HH11	1.84	0.41
1:A:661:SER:HB2	1:A:700:SER:HB3	2.01	0.41
1:C:819:PRO:HA	1:C:822:ASP:HB2	2.02	0.41
1:C:921:ASN:HB3	1:C:924:LEU:HB3	2.03	0.41
2:H:95:TYR:O	2:H:112:GLY:CA	2.68	0.41
1:A:330:ARG:HE	1:A:535:LEU:HD12	1.86	0.41
1:A:622:VAL:HA	1:A:625:ALA:HB3	2.01	0.41
1:B:332:PRO:HA	1:B:581:PRO:CB	2.51	0.41
1:C:100:ILE:HA	1:C:242:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:8:GLY:HA3	2:G:20:LEU:HD13	2.02	0.41
1:B:728:ILE:HG13	1:B:1063:VAL:HG23	2.02	0.41
1:C:642:SER:OG	1:C:643:ASN:N	2.53	0.41
3:K:107:LYS:HA	3:K:107:LYS:HD3	1.88	0.41
3:J:86:ALA:H	3:J:108:LEU:HB3	1.85	0.41
1:C:395:THR:HA	1:C:524:ALA:HA	2.02	0.41
1:C:1119:THR:HB	1:C:1142:PRO:HD2	2.02	0.41
1:A:144:LYS:HD2	1:A:144:LYS:HA	1.99	0.41
1:A:202:SER:HB2	1:A:225:LEU:HD23	2.03	0.41
1:C:331:PHE:HB3	1:C:530:LYS:HE2	2.01	0.41
1:C:982:ILE:HB	1:C:986:LEU:HD12	2.02	0.41
1:A:205:THR:HG22	1:A:207:ILE:H	1.86	0.41
1:B:64:TRP:HE1	1:B:266:ALA:HB1	1.85	0.41
1:B:298:LEU:HA	1:B:301:THR:HG22	2.03	0.41
1:B:305:LEU:HD12	1:B:310:VAL:HG12	2.03	0.41
1:B:323:GLN:HB2	1:B:630:GLN:HA	2.03	0.41
2:I:18:LEU:HB2	2:I:84:MET:HB3	2.02	0.41
3:J:19:THR:OG1	3:J:74:SER:OG	2.39	0.41
1:C:1154:LEU:HD23	1:C:1157:TYR:HD2	1.86	0.40
2:I:74:ASP:OD1	2:I:76:SER:OG	2.39	0.40
2:G:34:ALA:HB1	2:G:99:HIS:CE1	2.56	0.40
1:A:233:ASN:HB3	4:A:1302:NAG:HN2	1.87	0.40
1:A:312:LYS:HG2	1:A:666:ILE:HD11	2.04	0.40
1:A:446:LYS:HD3	2:H:60:ARG:HH21	1.86	0.40
1:C:145:ASN:HA	1:C:256:SER:HB2	2.04	0.40
3:K:63:ARG:O	3:K:78:SER:OG	2.36	0.40
1:C:921:ASN:O	1:C:925:ILE:N	2.54	0.40
2:H:3:THR:OG1	2:H:5:LYS:NZ	2.55	0.40
2:H:94:THR:HA	2:H:114:LEU:HA	2.04	0.40
1:A:98:SER:HA	1:A:175:ASP:HB2	2.04	0.40
1:B:500:ARG:O	1:B:502:THR:N	2.45	0.40
3:J:15:GLY:H	3:J:80:LEU:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1088/1270 (86%)	1017 (94%)	71 (6%)	0	100	100
1	B	1088/1270 (86%)	1017 (94%)	70 (6%)	1 (0%)	48	79
1	C	1088/1270 (86%)	1011 (93%)	77 (7%)	0	100	100
2	G	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	H	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	I	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
3	J	109/111 (98%)	99 (91%)	10 (9%)	0	100	100
3	K	109/111 (98%)	99 (91%)	10 (9%)	0	100	100
3	L	109/111 (98%)	99 (91%)	10 (9%)	0	100	100
All	All	3939/4497 (88%)	3676 (93%)	262 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	213	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	965/1113 (87%)	964 (100%)	1 (0%)	92	95
1	B	965/1113 (87%)	960 (100%)	5 (0%)	86	90
1	C	965/1113 (87%)	963 (100%)	2 (0%)	92	94
2	G	98/100 (98%)	97 (99%)	1 (1%)	73	80
2	H	98/100 (98%)	98 (100%)	0	100	100
2	I	98/100 (98%)	98 (100%)	0	100	100
3	J	90/91 (99%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	90/91 (99%)	90 (100%)	0	100	100
3	L	90/91 (99%)	90 (100%)	0	100	100
All	All	3459/3912 (88%)	3450 (100%)	9 (0%)	90	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	903	GLN
1	B	273	GLN
1	B	335	THR
1	B	396	ASN
1	B	446	LYS
1	B	583	THR
1	C	155	ARG
1	C	648	ARG
2	G	5	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	HIS
1	B	396	ASN
1	C	273	GLN
3	K	6	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

36 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1310	1	14,14,15	0.42	0	17,19,21	0.60	1 (5%)
4	NAG	B	1309	1	14,14,15	0.41	0	17,19,21	0.49	0
4	NAG	C	1312	1	14,14,15	0.39	0	17,19,21	0.53	0
4	NAG	A	1308	1	14,14,15	0.40	0	17,19,21	0.50	0
4	NAG	B	1301	1	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	B	1303	1	14,14,15	0.37	0	17,19,21	0.67	0
4	NAG	C	1309	1	14,14,15	0.35	0	17,19,21	0.51	0
4	NAG	A	1311	1	14,14,15	0.36	0	17,19,21	0.51	0
4	NAG	A	1307	1	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	C	1302	1	14,14,15	0.50	0	17,19,21	0.94	1 (5%)
4	NAG	B	1305	1	14,14,15	0.34	0	17,19,21	1.23	1 (5%)
4	NAG	B	1307	1	14,14,15	0.35	0	17,19,21	0.57	0
4	NAG	C	1305	1	14,14,15	0.44	0	17,19,21	0.52	0
4	NAG	B	1312	1	14,14,15	0.37	0	17,19,21	0.54	0
4	NAG	C	1303	1	14,14,15	0.33	0	17,19,21	0.49	0
4	NAG	C	1304	1	14,14,15	0.33	0	17,19,21	0.52	0
4	NAG	A	1309	1	14,14,15	0.36	0	17,19,21	0.53	0
4	NAG	A	1303	1	14,14,15	0.32	0	17,19,21	0.45	0
4	NAG	C	1311	1	14,14,15	0.35	0	17,19,21	0.51	0
4	NAG	B	1302	1	14,14,15	0.51	0	17,19,21	0.99	1 (5%)
4	NAG	B	1306	1	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	A	1305	1	14,14,15	0.38	0	17,19,21	0.62	0
4	NAG	B	1310	1	14,14,15	0.37	0	17,19,21	0.57	0
4	NAG	C	1301	1	14,14,15	0.34	0	17,19,21	0.50	0
4	NAG	A	1304	1	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	A	1312	1	14,14,15	0.87	1 (7%)	17,19,21	2.24	3 (17%)
4	NAG	B	1311	1	14,14,15	0.34	0	17,19,21	0.51	0
4	NAG	C	1306	1	14,14,15	0.38	0	17,19,21	0.52	0
4	NAG	B	1308	1	14,14,15	0.43	0	17,19,21	0.56	0
4	NAG	A	1301	1	14,14,15	0.38	0	17,19,21	0.50	0
4	NAG	B	1304	1	14,14,15	0.36	0	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1306	1	14,14,15	0.39	0	17,19,21	0.47	0
4	NAG	C	1310	1	14,14,15	0.46	0	17,19,21	0.49	0
4	NAG	C	1307	1	14,14,15	0.37	0	17,19,21	0.54	0
4	NAG	C	1308	1	14,14,15	0.35	0	17,19,21	0.51	0
4	NAG	A	1302	1	14,14,15	0.60	0	17,19,21	0.60	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1312	NAG	C1-C2	2.56	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1312	NAG	C2-N2-C7	7.80	134.02	122.90
4	B	1305	NAG	C2-N2-C7	3.69	128.16	122.90
4	A	1312	NAG	C1-C2-N2	3.62	116.67	110.49
4	C	1302	NAG	C2-N2-C7	3.11	127.33	122.90
4	B	1302	NAG	C2-N2-C7	2.99	127.16	122.90
4	B	1304	NAG	C1-O5-C5	2.76	115.93	112.19
4	B	1304	NAG	C4-C3-C2	-2.50	107.35	111.02
4	A	1310	NAG	C1-O5-C5	2.14	115.09	112.19
4	A	1312	NAG	C8-C7-N2	2.11	119.67	116.10
4	A	1302	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	C8-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
4	B	1305	NAG	C8-C7-N2-C2
4	B	1305	NAG	O7-C7-N2-C2
4	A	1311	NAG	C4-C5-C6-O6
4	C	1312	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1307	NAG	O5-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	A	1311	NAG	O5-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	C	1312	NAG	C4-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	B	1312	NAG	C4-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6
4	B	1305	NAG	C1-C2-N2-C7
4	A	1307	NAG	C4-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	A	1305	NAG	C8-C7-N2-C2
4	A	1305	NAG	O7-C7-N2-C2
4	A	1312	NAG	C8-C7-N2-C2
4	A	1312	NAG	O7-C7-N2-C2
4	A	1309	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6
4	A	1312	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	C	1310	NAG	C4-C5-C6-O6
4	A	1310	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	C	1310	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1307	NAG	O5-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	A	1312	NAG	C3-C2-N2-C7
4	B	1302	NAG	C3-C2-N2-C7
4	C	1302	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1302	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

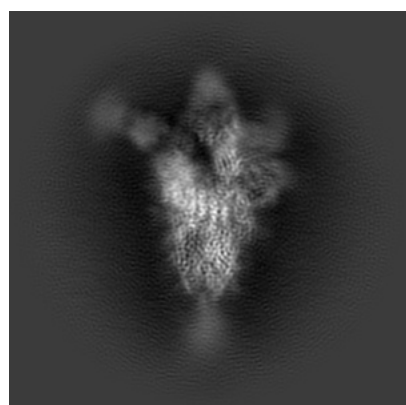
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32787. These allow visual inspection of the internal detail of the map and identification of artifacts.

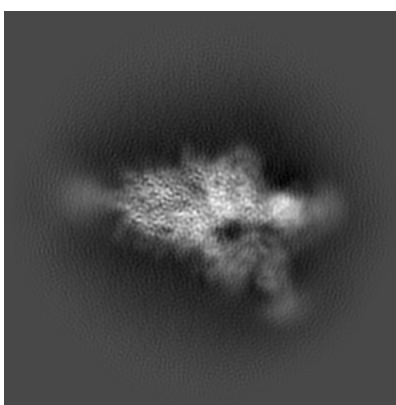
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

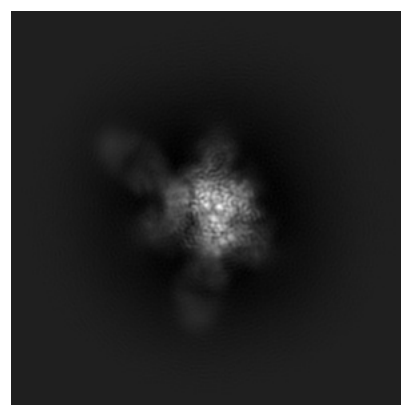
6.1.1 Primary map



X



Y

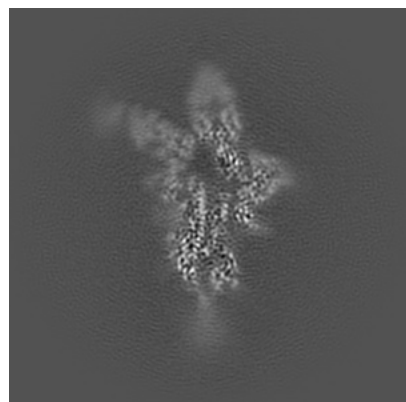


Z

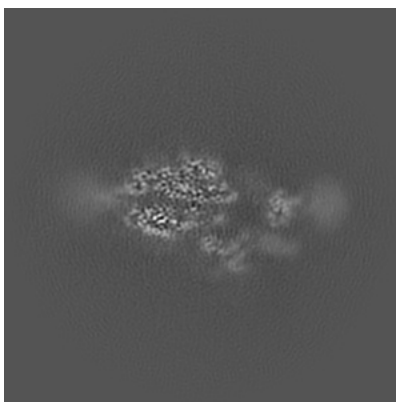
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

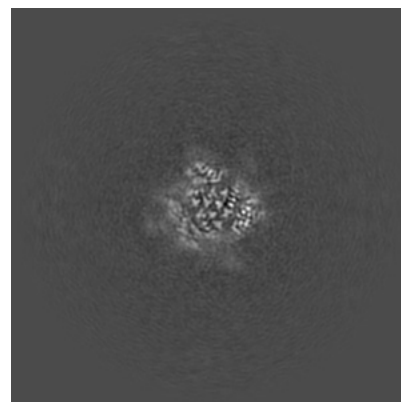
6.2.1 Primary map



X Index: 180



Y Index: 180

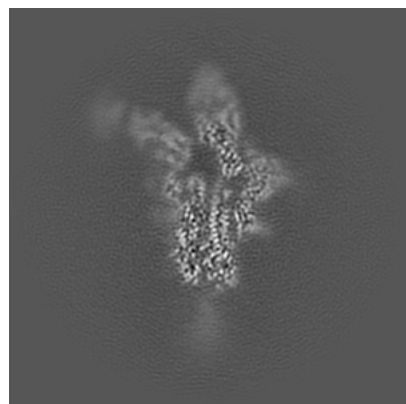


Z Index: 180

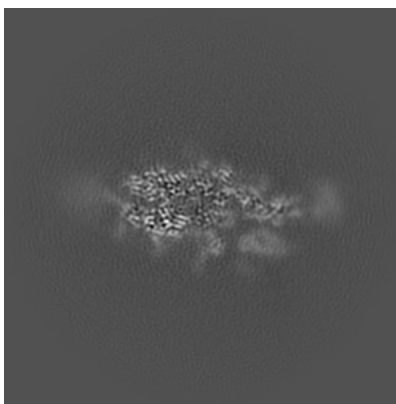
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

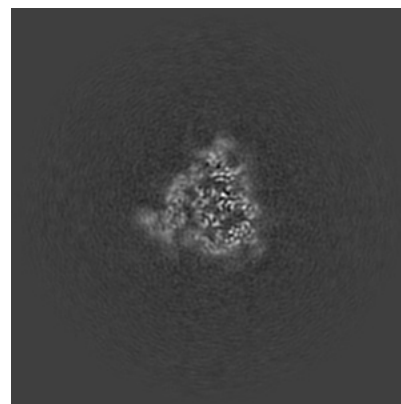
6.3.1 Primary map



X Index: 177



Y Index: 188

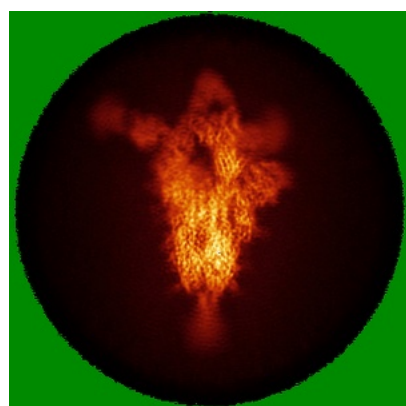


Z Index: 188

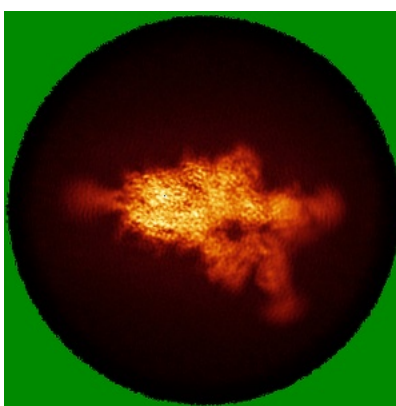
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

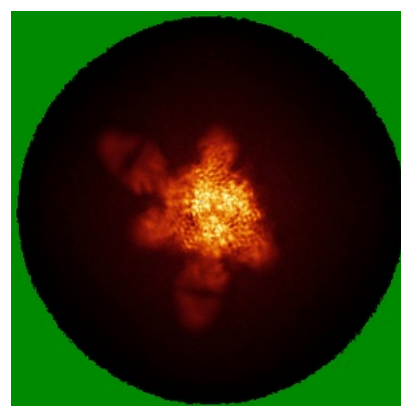
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

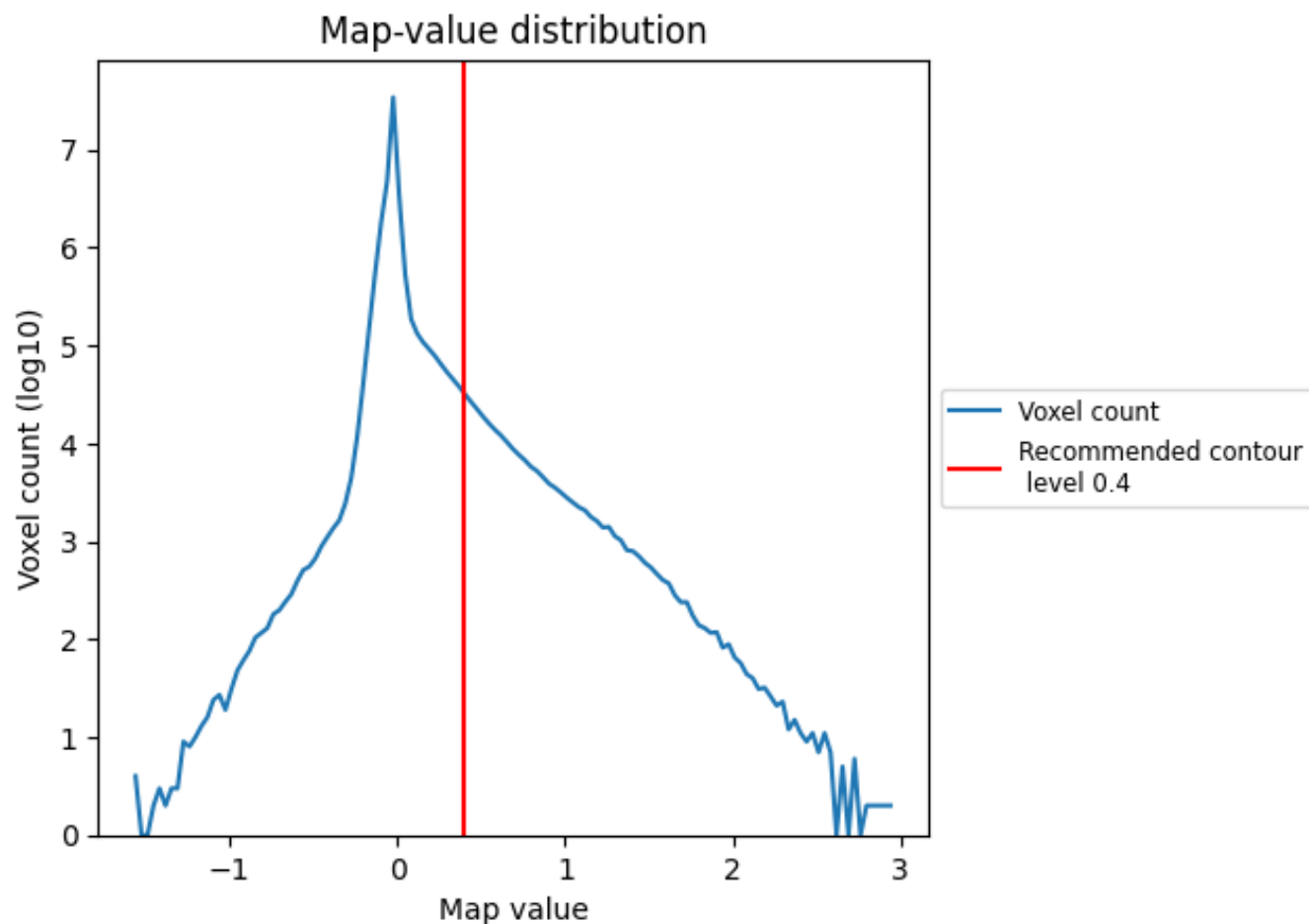
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

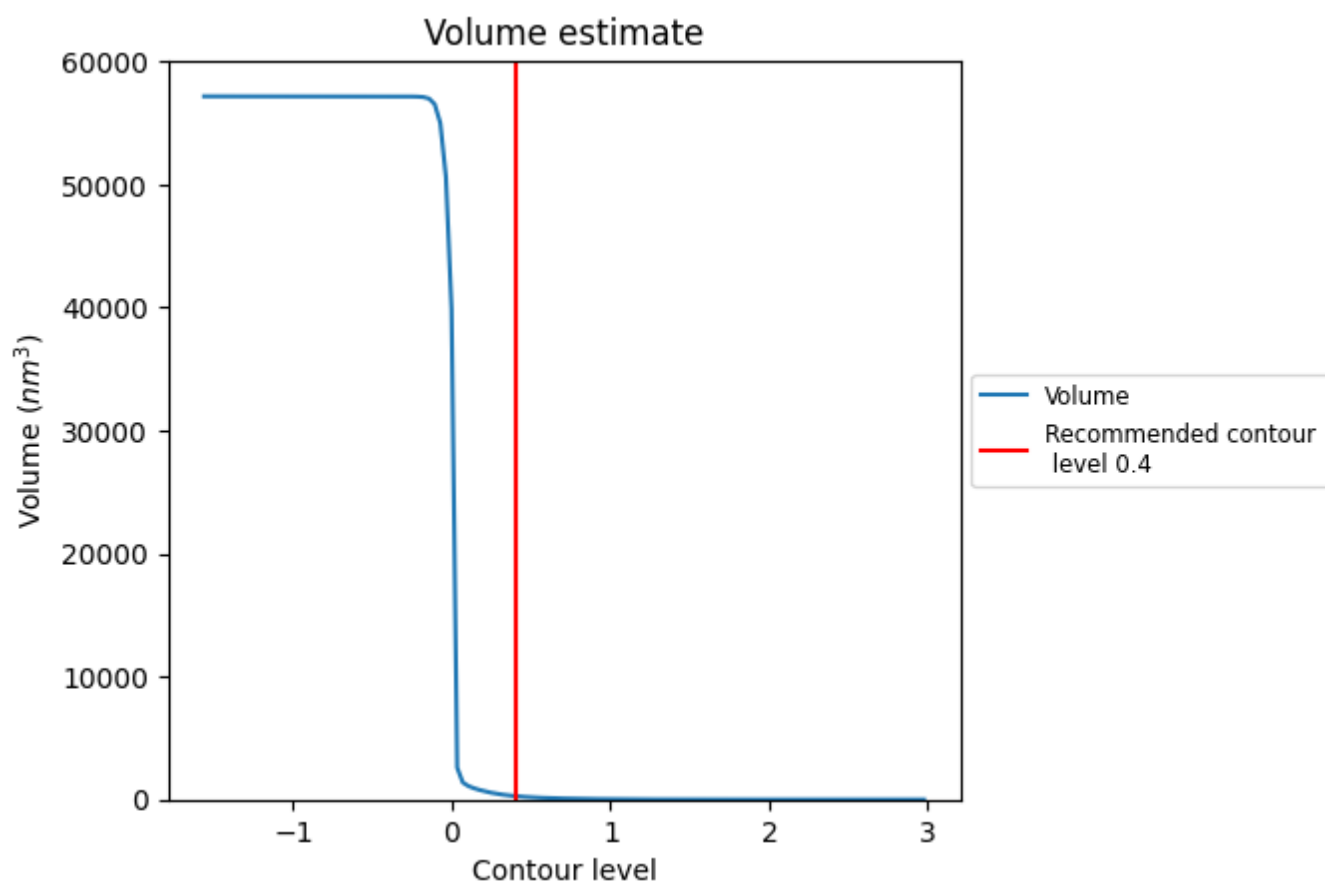
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

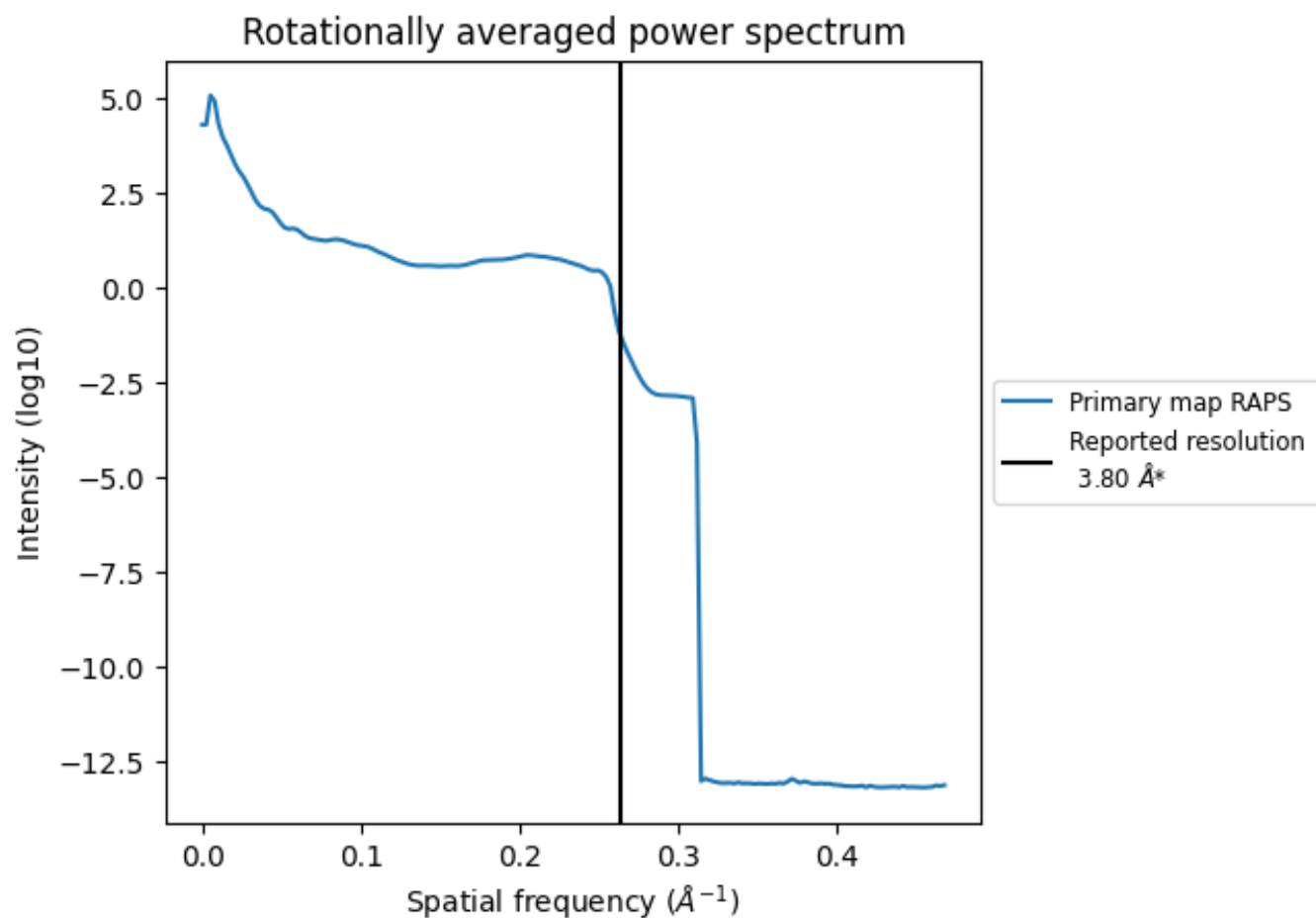
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm³; this corresponds to an approximate mass of 254 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

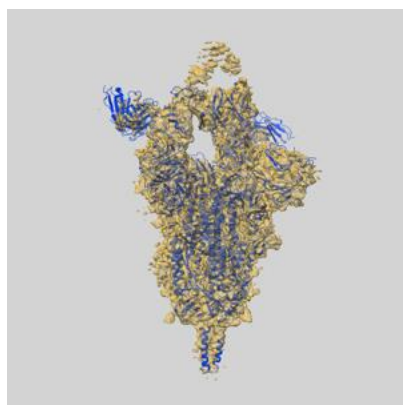
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

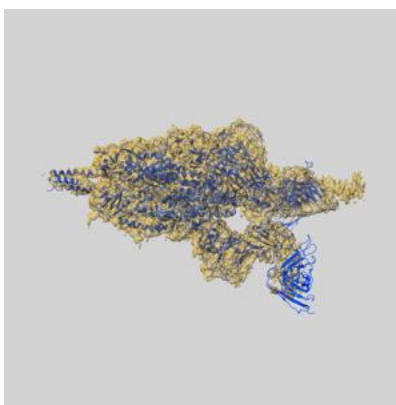
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32787 and PDB model 7WTI. Per-residue inclusion information can be found in section 3 on page 11.

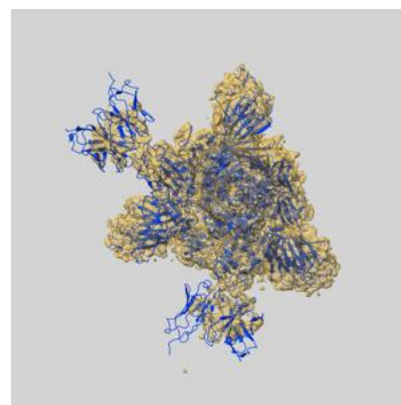
9.1 Map-model overlay [i](#)



X



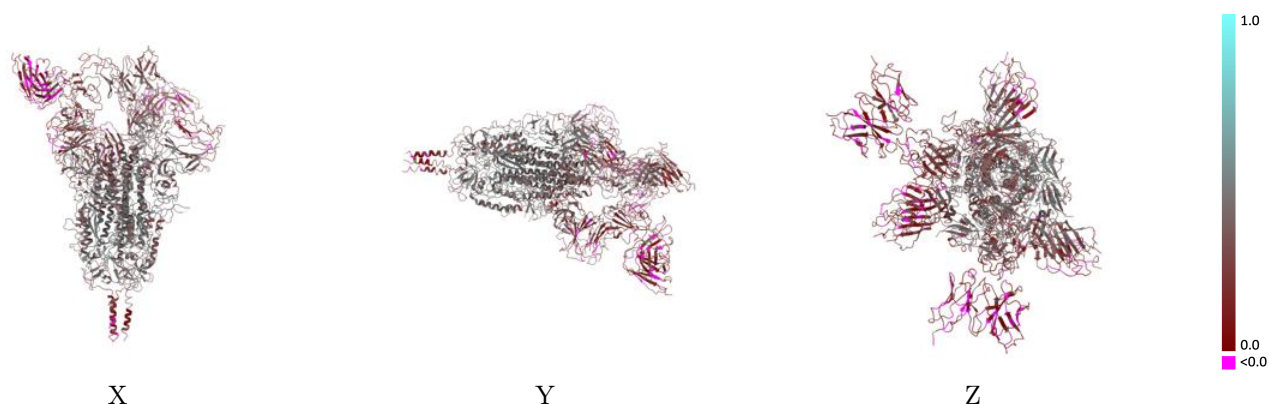
Y



Z

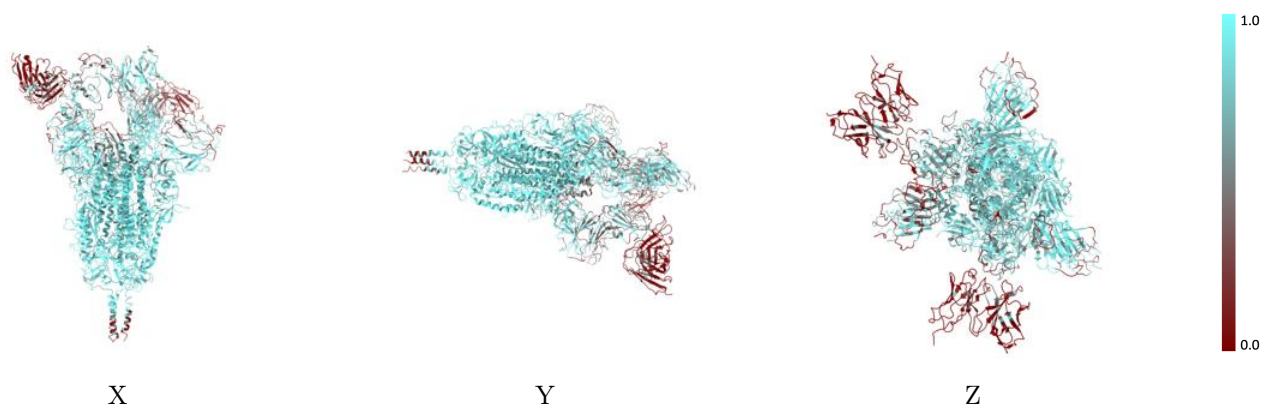
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



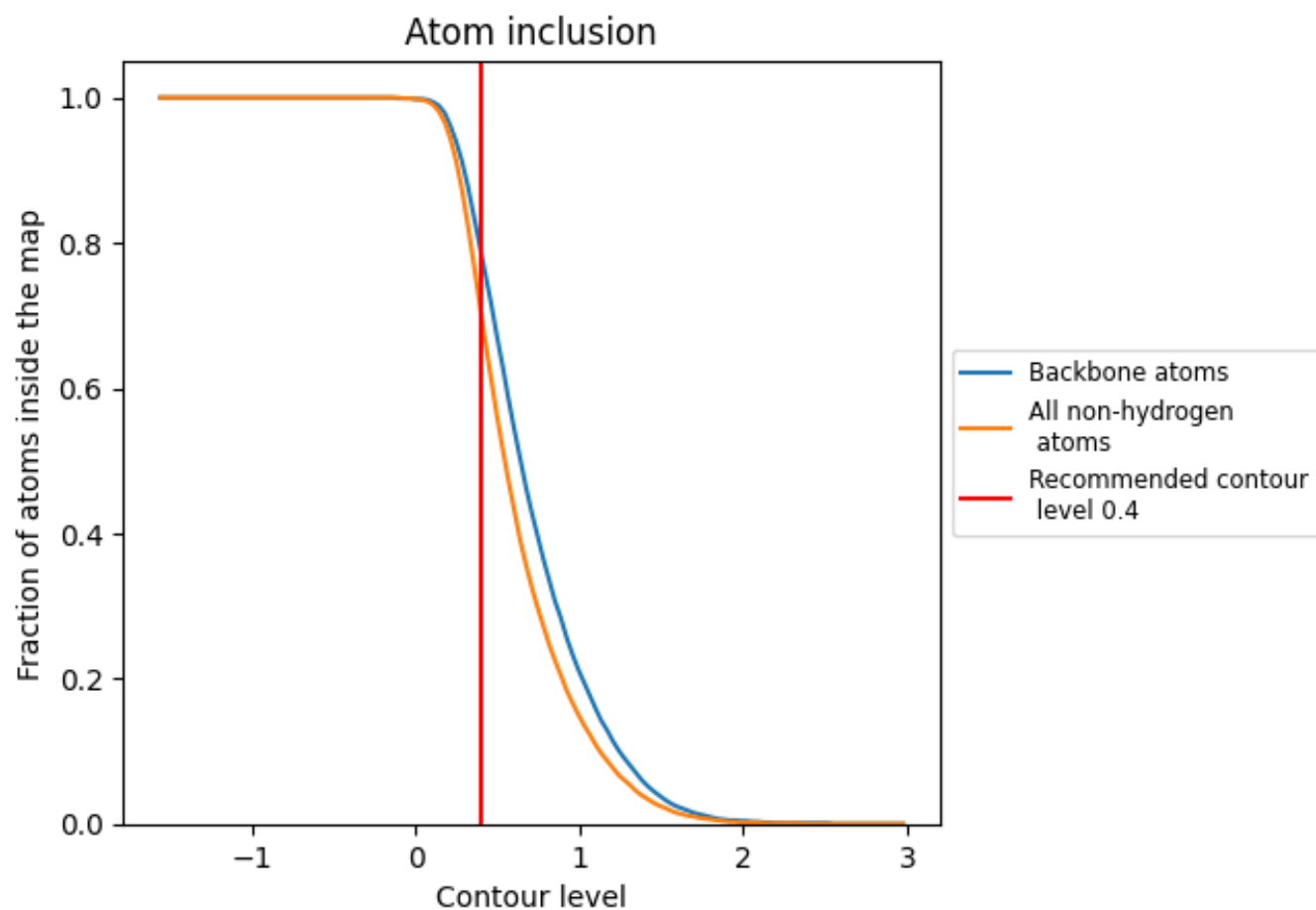
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6980	<div></div> 0.3220
A	<div></div> 0.8350	<div></div> 0.3820
B	<div></div> 0.7370	<div></div> 0.3250
C	<div></div> 0.7420	<div></div> 0.3360
G	<div></div> 0.1520	<div></div> 0.1040
H	<div></div> 0.7520	<div></div> 0.3010
I	<div></div> 0.1380	<div></div> 0.1260
J	<div></div> 0.0650	<div></div> 0.0980
K	<div></div> 0.0830	<div></div> 0.1690
L	<div></div> 0.7440	<div></div> 0.3430

1.0

0.0

<0.0